

An efficient method to compute the residual phase on a Lefschetz thimble

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We propose an efficient method to compute the so-called *residual phase* that appears when performing Monte Carlo calculations on a Lefschetz thimble. The method is stochastic and its cost scales linearly with the physical volume, linearly with the number of stochastic estimators and quadratically with the length of the extra dimension along the gradient flow. This is a drastic improvement over previous estimates of the cost of computing the residual phase. We also report on basic tests of correctness and scaling of the code.

I. INTRODUCTION

A Lefschetz thimble [1, 2] has been recently proposed as a tool to regularize quantum field theories (QFTs) and statistical systems (at least near criticality), in order to evade the infamous *sign problem* [3–7]. In the original proposal [3], one major difficulty of the approach was envisaged in the calculation of the so-called *residual phase*, that appears in the measure term when the thimble is not a flat manifold. This is a potential problem both because it threatens, in principle, to reintroduce a sign problem, and because its computation was expected to be very expensive (scaling like n^3 , where n is the number of degrees of freedom of the original system).

Actually, there are good reasons to expect that the residual phase does not reintroduce a sign problem, although they cannot be considered conclusive. First, the residual phase is completely neglected when one computes the asymptotic expansion around the saddle point that defines the thimble, which is expected to be a reasonable approximation in many cases. Second, the thimble does not oscillate unpredictably. Instead, its orientation smoothly interpolates between the directions of steepest descent at the saddle point (which are determined by the quadratic part of the action) and the asymptotic directions of convergence (which are determined by the highest degree of the interaction). In general, one can achieve very strange behaviors, by tuning the parameters of an action, but this is not expected to be the generic case. Third, the residual phase tends to deviate substantially from its value at the saddle point only on configurations that are correspondingly suppressed. Hence, we can expect that the thimble realizes a strong correlation between *phase* and *weight*, which is exactly what is missing on typical cases of difficult sign problem.

Although the previous arguments are merely qualitative, the best (and also quantitative) evidence that the residual phase does not reintroduce a sign problem is provided by the very precise computation performed in [6] for a complex scalar theory with ϕ^4 interactions in 4 dimensions. In fact, it was shown that the real part of the average residual phase is systematically larger than 0.99, for all the parameter values studied there¹. None of these considerations allows us to conclude that the residual phase will not introduce a sign problem in other regimes or other models. However,

¹ It is worthwhile noting that the residual phase introduces sizable corrections when one considers the same action, but in zero dimensions [8, 9]. Although a precise comparison is impossible, this suggests a suppression of the contribution of configurations with large residual phases in presence of many degrees of freedom.

they are certainly sufficient to motivate further investigation of this approach, including the search for more efficient strategies to compute the residual phase.

In this paper, we first review how the residual phase appears in the Lefschetz thimble approach, and then we propose a new method to compute it numerically, with much better scaling properties than the naive method proposed in [3]. The method exploits the properties of the thimble and standard numerical techniques. In particular, we compute a trace over space-time indices with stochastic estimators, which ensure acceptable computational costs and easy parallelization. Finally, we present some basic tests of the new method on small lattices.

II. DEFINITION OF THE RESIDUAL PHASE

In order to understand how the residual phase appears in an integration on a Lefschetz thimble, consider the integral:

$$\int_{\mathbb{R}^n} f(x) \prod_{i=1}^n dx_i. \quad (1)$$

The Lefschetz thimble approach leads us to complexify $f(x)$ into $f(z)$, with $z \in \mathbb{C}^n$, and substitute formula (1) with the integral (see Eq. (1) of [1]):

$$\int_{\Gamma} f(z) dz_1 \wedge \dots \wedge dz_n, \quad (2)$$

where Γ is a Lefschetz thimble, and $d^n z := dz_1 \wedge \dots \wedge dz_n$ is a form of precisely the right degree to integrate a manifold of real dimension n in \mathbb{C}^n , as it is indeed the dimension of the manifold Γ . (Note that $d^n z$ is not the standard volume form in \mathbb{C}^n , which is, instead, $dz_1 \wedge d\bar{z}_1 \wedge \dots \wedge dz_n \wedge d\bar{z}_n$.)

In a generic point $\zeta \in \Gamma$, the form $d^n z$ and the tangent space $T_{\zeta}\Gamma$ are not parallel. In order to evaluate the integral (2), we need to express it as an ordinary integral in \mathbb{R}^n . To this end, we must change the coordinates from the canonical basis of \mathbb{C}^n (dual to the forms dz_i , $i = 1 \dots n$) into a basis of $T_{\zeta}\Gamma$ (let us call such basis $u^{(1)}, \dots, u^{(n)}$)². Let U be the $n \times n$ complex matrix whose columns are the vectors of the basis $u^{(i)}$.

The change of basis can be realized, locally, with a chart $\varphi : N \subset \Gamma \rightarrow \mathbb{R}^n$, defined on a neighborhood $N \subset \Gamma$ of ζ . For instance, we can define φ as:

$$\varphi(\zeta + \sum_i u^{(i)} y_i) = y + O(y^2) \in \mathbb{R}^n. \quad (3)$$

Then the integral (2) becomes:

$$\int_N f(z) dz_1 \wedge \dots \wedge dz_n = \int_{\varphi(N)} f(\varphi^{-1}(y)) \det U(\varphi^{-1}(y)) \prod_i dy_i. \quad (4)$$

The integral (4) can be performed by Monte Carlo methods. For this, we need to sample the points in Γ uniformly according to the measure induced by the standard hermitian metric of \mathbb{C}^n (equivalently, the Euclidean metric in \mathbb{R}^{2n}), while taking into account the determinant of U . In the algorithm of [3], the metric enters only in the computation of the length of the random noise vectors, where, indeed, the Euclidean metric in \mathbb{R}^{2n} is used. This ensures that this algorithm samples Γ uniformly according to the correct measure. Therefore, we are left with the computation of $\det U$, which is the topic of the rest of this paper³.

² We will see, in the next section, that this can be accomplished through a unitary transformation

³ Note that in [5] the residual determinant is not exactly the same as the one defined above. In [5] the manifold Γ is explored by making proposals that are uniform in the variables $\eta \in \mathbb{R}^n$, that diagonalize and rescale the quadratic part of the action. Therefore, the residual Jacobi *determinant* in that case is:

$$\det(\mathbf{J}_{\eta}^{\phi}) = \det\left(\frac{\partial \phi}{\partial \eta}\right), \quad (5)$$

which is different from $\det U$ in Eq. (4), and it is not a phase, in general.

III. TANGENT SPACE AT THE SADDLE POINT

It is important to observe that there is a special matrix $J \in M(\mathbb{R}^{2n})$ (almost complex structure) that represents, in \mathbb{R}^{2n} , the multiplication by i in \mathbb{C}^n . Its form is:

$$J = \begin{pmatrix} 0 & 1_n \\ -1_n & 0 \end{pmatrix}. \quad (6)$$

The matrix J anti-commutes with the Hessian⁴ $H(z) = \partial_{i,j}^2 S_R(z)$ for each z . This implies that J transforms any eigenvector of $H(z)$ with eigenvalue λ into another eigenvector with eigenvalue $-\lambda$.

The thimble is well defined only if the Hessian is non-degenerate at the saddle point ζ_0 , and we assume that this is the case in the following. Let V_+ be the $2n \times n$ real matrix whose columns are the eigenvectors of $H(\zeta_0)$ with positive eigenvalues and define

$$V_- := JV_+. \quad (7)$$

We can define a matrix U_+ by the n complex column vectors: $u_h^{(i)} := v_{R,h}^{(i)} + iv_{I,h}^{(i)}$, $i, h = 1, \dots, n$. In matrix notation we can write:

$$U_+ = PV_+, \quad P = (1_n, i_n). \quad (8)$$

Now U_+ is unitary. In fact,

$$\begin{aligned} \sum_h \bar{u}_h^{(i)} u_h^{(j)} &= \sum_h (u_{R,h}^{(i)} - iu_{I,h}^{(i)})(u_{R,h}^{(j)} + iu_{I,h}^{(j)}) = \sum_h (u_{R,h}^{(i)} u_{R,h}^{(j)} + u_{I,h}^{(i)} u_{I,h}^{(j)} + i(u_{R,h}^{(i)} u_{I,h}^{(j)} - u_{I,h}^{(i)} u_{R,h}^{(j)})) \\ &= (v^{(i)})^2 + i(v^{(i)} J v^{(j)}). \end{aligned}$$

The last imaginary term vanishes because V_+ is orthogonal to JV_+ .

What we have shown is sometimes expressed by the relation $U(n) \simeq SO(2n) \cap Sp(2n)$. In [6] it is called *reality condition*.

IV. EVOLUTION OF THE TANGENT SPACE

The orthogonality of V_+ and $V_- := JV_+$ is preserved by the evolution⁵. In fact,

$$V_+(\tau + d\tau) = V_+(\tau) + d\tau H(z(\tau)) V_+(\tau), \quad (9)$$

then

$$\begin{aligned} V_+^T(\tau + d\tau) J V_+(\tau + d\tau) &= V_+^T(\tau) J V_+(\tau) + d\tau [V_+^T(\tau) J H(z(\tau)) V_+(\tau) + V_+^T(\tau) H(z(\tau))^T J V_+(\tau)] \\ &= 0 + d\tau [V_+^T(\tau) \{J, H\} V_+(\tau)] = 0. \end{aligned}$$

On the other hand, $V_+(\tau + d\tau)$ and $V_-(\tau + d\tau)$ are not orthonormal anymore. If we orthonormalize them (e.g. with Gram-Schmidt, as it is done in [6]), we obtain a new basis $V_+^I(\tau + d\tau)$, such that

⁴ We use i, j for multi-indices that include also the real/imaginary part of z , for all n degrees of freedom. Hence, $H(z)$ is a $2n \times 2n$ real symmetric matrix

⁵ Note that the evolved matrix $V_+(\tau)$ is *not* a basis of the eigenvectors of the Hessian $H(z(\tau))$, computed in the evolved configuration $z(\tau) \in \Gamma$.

$V_+ = V'_+ W$, with W $n \times n$ and upper triangular. Then we can use the projector P , defined in Eq. (8), to define the matrix $U_+(\tau + d\tau) := PV'_+(\tau + d\tau)$. Now $U_+(\tau)$ is unitary for all τ , in fact:

$$P^\dagger P = 1_{2n} + iJ, \quad (10)$$

$$\begin{aligned} (PV'_+)^{\dagger}(PV'_+) &= (V'_+)^T (P^\dagger P) (V'_+) = (V'_+)^T (1_{2n} + iJ) (V'_+) = \\ &= (V'_+)^T 1_{2n} (V'_+) + i(V'_+ W^{-1})^T J (V'_+ W^{-1}) = 1_{2n} + 0. \end{aligned} \quad (11)$$

In particular $\det(U_+) = e^{i\phi}$ and we have shown that the residual phase is actually a phase.

V. EVOLUTION BY CONTINUOUS ORTHOGONALIZATION

Instead of evolving the vectors in $V_+(\tau)$ with Eq. (9), we can combine evolution and orthonormalization at every step as prescribed by the Drury-Davey [10, 11] method of continuous orthogonalization (see also [12] for a nice geometrical discussion and generalization). The evolution equation, with Euler method, is:

$$\begin{aligned} V_+(\tau + d\tau) &= V_+(\tau) + d\tau(1 - V_+(\tau)V_+(\tau)^T)H(z(\tau))V_+(\tau) = \\ &= V_+(\tau) + d\tau(V_-(\tau)V_-(\tau)^T)H(z(\tau))V_+(\tau). \end{aligned} \quad (12)$$

It is straightforward to check that, at all times τ , both the vectors V_+ and V_- remain orthonormal and orthogonal to each other:

$$V_+(\tau)^T V_+(\tau) = 1_n, \quad (13)$$

$$V_-(\tau)^T V_-(\tau) = (JV_+(\tau))^T (JV_+(\tau)) = 1_n, \quad (14)$$

$$V_+(\tau)^T V_-(\tau) = V_+(\tau)^T JV_+(\tau) = 0. \quad (15)$$

Now we can define a unitary matrix directly from $V_+(\tau)$:

$$U_+(\tau) = PV_+(\tau). \quad (16)$$

Eq. (12) implements an Iwasawa projection (equivalently, a Gram-Schmidt infinitesimal orthonormalization) at every τ , but it is much more expensive than Eq. (9)⁶. In fact, the cost of implementing Eq. (12) scales like n^3 . Eq. (12) will be used, in the next section, to deduce a simple formula for the residual phase, but eventually it will not be needed in the method that we propose. We will use Eq. (12) only to cross-check the results obtained with our method.

VI. COMPUTING THE RESIDUAL PHASE

After the preparatory analysis of the previous sections, we come to the formula for the computation of the residual phase, that is the main result of this paper. We can assume to know the phase ϕ_0 at the stationary point, and we can also assume that this is attained for $\tau = \tau_0$ sufficiently

⁶ Note that the evolution defined by Eq. (6) of [13] is not correct. In order to ensure an orthogonal evolution one should use instead Eq. (12) above.

large (i.e., $\det U_+(\tau_0) = e^{i\phi_0}$). Therefore,

$$\begin{aligned}
\log \det U_+(\tau) &\stackrel{\text{Eq. (16)}}{=} \log \det [PV_+(\tau)] = \text{Tr} \log [PV_+(\tau)] = \\
&= \int_{\tau_0}^{\tau} ds \text{Tr} \left[(PV_+(s))^{-1} P \frac{dV_+(s)}{ds} \right] + i\phi_0 \\
&\stackrel{U_+ \text{ unitary}}{=} \int_{\tau_0}^{\tau} ds \text{Tr} \left[(PV_+(s))^{\dagger} P \frac{dV_+(s)}{ds} \right] + i\phi_0 \\
&= \int_{\tau_0}^{\tau} ds \text{Tr} \left[V_+(s)^T (P^{\dagger} P) \frac{dV_+(s)}{ds} \right] + i\phi_0 \\
&\stackrel{\text{Eq. (10)}}{=} \int_{\tau_0}^{\tau} ds \text{Tr} \left[V_+(s)^T (1_{2n} + iJ) \frac{dV_+(s)}{ds} \right] + i\phi_0 \\
&\stackrel{\text{Eq. (12)}}{=} \int_{\tau_0}^{\tau} ds \text{Tr} [V_+(s)^T (1_{2n} + iJ) (V_-(s) V_-(s)^T H(s) V_+(s))] + i\phi_0 \\
&\stackrel{\text{Eq. (15)}}{=} i \int_{\tau_0}^{\tau} ds \text{Tr} [V_+(s)^T J V_-(s) V_-(s)^T H(s) V_+(s)] + i\phi_0 \\
&\stackrel{\text{Eq. (7)}}{=} i \int_{\tau_0}^{\tau} ds \text{Tr} [V_+(s)^T J^2 V_+(s) V_+(s)^T J^T H(s) V_+(s)] + i\phi_0 \\
&\stackrel{J^2 = -1, J^T = -J}{=} (-1)^2 i \int_{\tau_0}^{\tau} ds \text{Tr} [V_+(s)^T V_+(s) V_+(s)^T JH(s) V_+(s)] + i\phi_0 \\
&\stackrel{\text{Eq. (13)}}{=} i \int_{\tau_0}^{\tau} ds \text{Tr} [V_+(s)^T JH(s) V_+(s)] + i\phi_0.
\end{aligned}$$

Note that the result is purely imaginary, which confirms that the residual phase in this setup is indeed a phase⁷. As a result, we have to compute the trace of the operator $JH(z)$ on the tangent space $T_z\Gamma$.

For very large n it should be convenient to use a stochastic estimator of the trace, rather than compute it fully. Using N_R random noises, we have:

$$\text{Tr} [V_+(s)^T JH(s) V_+(s)] = \lim_{N_R \rightarrow \infty} \frac{1}{N_R} \sum_{r=1}^{N_R} \xi^{(r)T} V_+(s)^T JH(s) V_+(s) \xi^{(r)}. \quad (17)$$

Note that the vectors $\eta^{(r)}(s) = V_+(s) \xi^{(r)}$ are generic random vectors in $T_{z(s)}\Gamma$. One way to compute Eq. (17) is by extracting random vectors $\eta^{(r)}(s) \in \mathbb{C}^n$, evolve them as usual down to τ_0 along the curve $z(\sigma)$, $\sigma \in [s, \tau_0]$, project them with the free projector, evolve them back to s and compute

$$\frac{1}{N_R} \sum_{r=1}^{N_R} \eta^{(r)T}(s) JH(s) \eta^{(r)}(s).$$

The evolution back and forth ensures the isotropy of the distribution of the η [3]. But, note that we have to generate η for each s . The final formula is therefore:

$$\log \det U_+(\tau) - i\phi_0 = \lim_{N_R \rightarrow \infty} i \int_{\tau_0}^{\tau} ds \frac{1}{N_R} \sum_{r=1}^{N_R} \eta^{(r)T}(s) JH(s) \eta^{(r)}(s). \quad (18)$$

The costs of computing Eq. (18) scales as $n \times N_{\tau}^2 \times N_R$, where N_{τ} is the number of steps in which the dimension along the gradient flow is subdivided. This cost is a drastic improvement over what we had estimated in [3]. Of course, one expects that the required N_R will increase linearly with n , but the experience with stochastic estimators tells that it is usually sufficient to use $N_R \ll n$.

⁷ Note also that the inverse matrix that appears in [13] has disappeared here, because the matrix $U_+(s)$ (called T_{ϕ_s} in [13]) is actually unitary.

VII. NUMERICAL TESTS

In order to test our method, we implemented two algorithms. One code computes the residual phase as defined in Eq. (18), in the previous section (hereafter called *stochastic* method). Another code computes the residual phase by evolving the basis $V_+(\tau)$ with Eq. (12) and then computes the determinant with the lapack function `zgeevx` [14] (hereafter called the *exact* method). The exact method has of course very limited applicability, as it scales as $O(n^3)$ (although it scales linearly with N_τ) and it is hardly parallelizable. The exact method is used here only to test the stochastic method⁸.

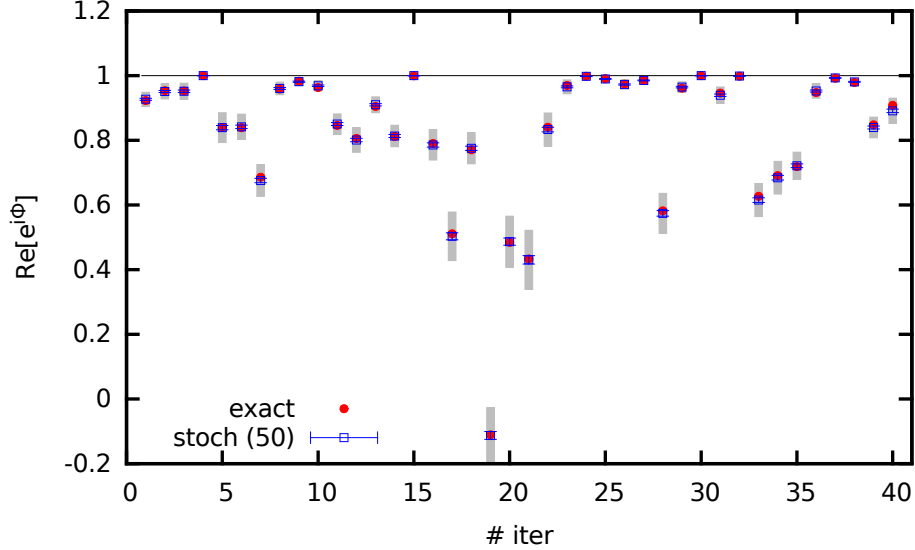


FIG. 1. Comparison of the computation of the residual phase with the *exact* and with the *stochastic* method. Here we show the real part of the residual phase for a small sample of configurations that belong to the same Monte Carlo sequence (the iteration number is shown in the horizontal axis). The blue errorbars are obtained by using $N_R = 50$ stochastic estimators. On the other hand, the grey band shows the standard deviation, which indicates the distribution that a single stochastic estimator would have. The other parameters of the simulation are $n = 2 \times 16^2$, $N_\tau = 64$, $\mu = 1.05$, $m = \lambda = 1$, $\Delta\tau = \Delta t_{Langevin} = 10^{-3}$. See [4] for the meaning of the parameters which are not defined here. Note that the configurations shown here are not typical of their ensemble: no attempt is made here to compute reliably the *average* residual phase for any ensemble.

In order to test the method, we have applied it to the usual complex scalar field with ϕ^4 interaction and with chemical potential [4]. Here we limit ourself to a two dimensional system, in order to sample very cheaply different lattices sizes.

As a test of correctness, in Fig. 1 we compare the results of the two methods on a set of configurations. The test is passed brilliantly. Moreover, the grey bands in Fig. 1 display the standard deviation of the stochastic method; this is the statistical error that we expect if only one source is used. The size of the standard deviation indicates that even a single stochastic source is able to yield a fairly accurate estimate in these cases. As one can expect, the standard deviation is larger when the residual phase differs more from its value at the saddle point, but the stochastic method seems always reliable.

⁸ The method employed in [6] is similar to our exact method, but uses the evolution defined by Eq. (9), and integrated with the fourth-order Runge-Kutta scheme, rather than Eq. (12). The method of [6] is probably the best compromise on small lattices, but, on large lattices, it is expected to scale less favorably than the stochastic method presented here.

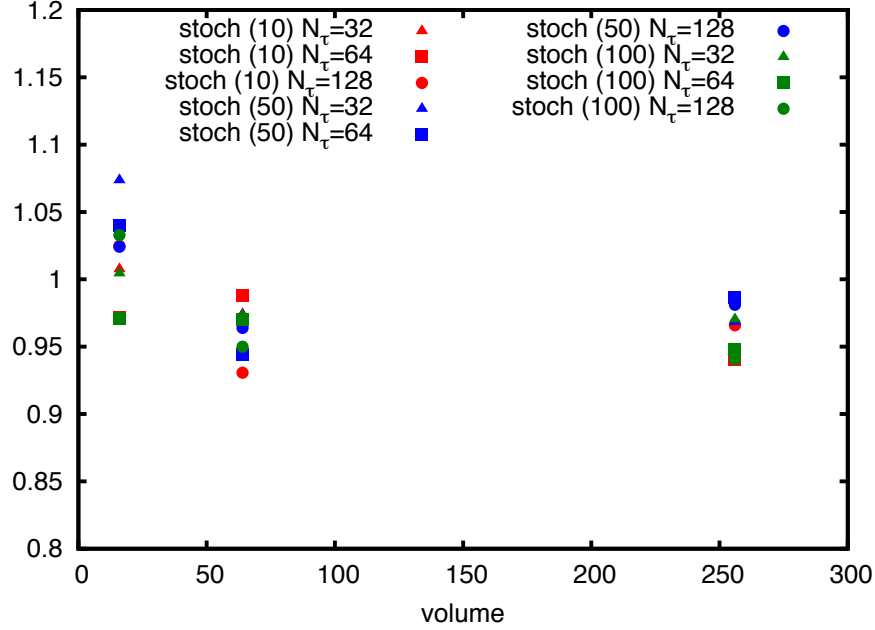


FIG. 2. Scaling of the costs to compute the residual phase with the stochastic method. The plot compares the actual cost with the estimate based on the scaling $O(n \times N_\tau^2 \times N_R)$, and normalized at the point with $n = 2 \times 4^2$, $N_R = 1$, $N_\tau = 32$. The other parameters are the same as in the previous plot.

Besides these tests of correctness, we also tested the expected scaling of the computational costs (although still on small lattices). Fig. 2 shows that, as expected, the costs of the stochastic method scale as $O(n \times N_\tau^2 \times N_R)$. In these very small lattices, the exact and stochastic methods still have roughly comparable costs: for example, for $N_\tau = 128$ and $n = 2 \times 16^2$, the exact method costs as much as the stochastic one with $N_R \simeq 80$. However, the stochastic method will necessarily become more efficient on larger systems. It is difficult to tell how the number of stochastic estimators N_R will scale on large systems, when keeping the precision of the computation of the residual phase fixed. Generically, one expects a volume dependence also in N_R , but the fact that $N_R = 1$ seems already sufficient here is very encouraging.

In this paper, we did not try to estimate the *average* residual phase for any ensemble. This paper is only concerned with the proposal and the testing of a new method to compute the residual phase efficiently and precisely on a given configuration. In particular, the configurations in Fig. 1 are not typical of their ensemble. Of course, it will be eventually very interesting to see how the average residual phase scales on larger volumes and for realistic systems, and how it depends on the technical parameters that describe the thimble. These will be the crucial questions when studying a specific physical system, but they go beyond the scope of the present paper.

VIII. CONCLUSIONS

In this paper we have proposed a new method to compute the residual phase that appears on Monte Carlo calculations on a Lefschetz thimble. In particular, our main result is the derivation of the formula in Eq. (18). By this, we have also corrected a mistake in [13]. Moreover, we have reported the results of the testing of our code and we have also verified the expected scaling of the costs as $O(n \times N_\tau^2 \times N_R)$. A further advantage of the stochastic method is the fact that it can be easily parallelized across the physical volume (our code is indeed already parallel). The fact that already one single stochastic estimator seems to be sufficient in these tiny lattices is certainly not

conclusive, but quite encouraging.

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